

National Center for Computational Sciences (NCCS) Snapshot July 10, 2006

NCCS Systems

On Monday, July 3rd, the NCCS reached another milestone. The High-Performance Storage System (HPSS) passed 1 petabyte of stored data. HPSS allows researchers to store and rapidly access data from their simulations. HPSS has been in production at Oak Ridge National Laboratory (ORNL) since 1997 and continues to be developed and enhanced. The ability to store large amounts of data is an invaluable tool for research teams, particularly as the sizes of the NCCS computers and the simulations run on the machines continue to grow and produce breakthrough science.

Exciting improvements are being made to other NCCS systems as well. The upgrade of the Cray XT3 (Jaguar) operating system to version 1.4.19 was completed last week. This software release is required for the dual-core upgrade to be performed later this month. The cutting-edge dual-core technology fits two processor cores on a single die and will give users of the system double the current processing capacity with minimal increases in power consumption and heat levels.

In addition, the operating system for the Cray XT3 development system (Rizzo) was upgraded to version 1.4.19 and the hardware was upgraded to dual-core, and applications testing began with the dual-core Catamount operating system. Members of the NCCS staff are now beginning to perform applications testing with compute-node Linux.

SciDAC (Scientific Discovery through Advanced Computing) Conference

The 2006 SciDAC Conference was held in Denver, Colorado, on June 25–29. Several researchers with Leadership Computing Facility (LCF) allocations were on hand at the conference to present their findings to the computational science community. These scientists represented a wide variety of disciplines, including astrophysics, chemistry, materials science, and accelerators, demonstrating again that the resources of the NCCS are enabling breakthrough science in many fields. An overarching theme of the conference was the move toward petascale computing in the near future and the impact the change will have on science. The NCCS is prepared to lead the way on the road to petascale computing as a part of the LCF Project, which will see a petascale machine installed by late 2008.

Computational Science Graduate Fellowship Conference

The 2006 Department of Energy (DOE) Computational Science Graduate Fellowship Annual Fellows' Conference was held in Washington, D.C., on June 20–22. Managed by the Krell Institute for the past 10 years, the annual conference makes it possible for leaders and students to gather, network, and discover the research opportunities at DOE laboratories. The Computational Science Graduate Fellowship program supports a remarkably talented pool of young computational scientists who are required to perform at least one 12-week practicum at a DOE lab during their 4-year fellowship tenure. The costs of the practicum are wholly borne by the fellowship program through the Krell Institute. The 2006 conference hosted nearly 100 students.

The NCCS had a more visible presence at this year's conference than ever before. A new poster highlighted ORNL and the science that is being accomplished as a result of the resources that are available to researchers here at the NCCS. In addition, two staff members, Bronson Messer and Richard Mills, attended the conference to interact with the students. As a result, they effectively recruited several of the first- and second-year fellows to come to ORNL to perform their required practicums. These students come from a wide variety of backgrounds, including astrophysics, chemistry, and materials science.